A Note on the Nuclear Excited Feshbach Resonance

H. S. Desai

Department of Physics, M. S. University of Baroda,
Baroda (Gujarat), India

M. P. Maru

Physics Department, D. K. V. Arts and Science College,
Jamnagar (Gujarat), India

and S. R. Pandya

Department of Physics, M. S. University of Baroda,
Baroda (Gujarat), India

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The scattering amplitude and the wave function for the final bound state of an electron in Turner's[1] mechanism are modified. The life time for the temporarily formed negative ion and the capture cross section in the case of electron-polar molecule interaction are reported.

It is observed that the effect of our modification is to increase the life time and to decrease the capture cross section. Our results favour the existence of long lived parent negative ions.

In spite of the large amount of work done on the subject of the scattering of slow electrons by polar molecules there still exists a controversy regarding the large diffusion cross section of some of the polar molecules. In order to explain the large scattering cross section Turner[1] proposed that there exists a momentary capture of the slow electron with a rotational excitation of the polar molecule. It is well known that, though this was a major breakthrough, some facts about the large capture time remain unexplained. Recently, Christophorou[2–4] has reported that the life time of negative ions in the captured state is much larger than predicted theoretically. Calculations were also made by Itikawa[5] for the cross section of electron scattering by polar molecules, taking into account the capture and decay processes in unified manner. The large cross section may also be attributed to short range forces[6, 7]. However, recent experiments[2–4] favour the Feshbach type resonance as predicted by Turner.

In this short communication we have made an attempt to find out the consequences of using simultaneously a better approximation for the scattering amplitude and a slightly different wave function for the bound state of the electron in the dipole field. Our corrections favour the existence of long lived negative parent ions.

For the determination of the scattering amplitude the variational method as established by Mower[8] on the basis of the variational method developed by Schwinger[9], is used. The expression for the trial wave functon needed in this method is of the form Ce^{iks}. By the use of this trial function the scattering amplitude is obtained as

$$f(\theta) = f_B(\theta)\,[1 + T_0(\theta)]\,. \qquad (1)$$

$f_B(\theta) = 2\,i\,D\,e\,m\,\nu'/\hbar^2 k$ is the amplitude using the Born approximation and $T_0(\theta) = (i\,k/2)\,f_B(\theta)$, where m is the mass of the electron. ν' is the direction cosine of the dipole with respect to the wave vector **K**. The magnitude of $\boldsymbol{K}$ is given by $K_0[2(1-\cos\theta)]^{1/2}$. θ is the angle between the initial and the scattering direction. It is observed that the use of the trial function gives an amplitude factor slightly larger than the Born approximation scattering amplitude $f_B(\theta)$. The diffusion cross section also increases.

For the final bound state we choose a wave function of the electron which is the sum of the S and P states as given by[1] but differing from that in the radial part. Thus, we write a trial function for the final bound state of the electron

$$\psi_f = \frac{N}{1+p^2\zeta^2}\,\{C_0\,Y_{00}(\theta,\Phi) + C_1\,Y_{10}(\bar\theta,\Phi)\} \qquad (2)$$

where N is the normalization constant and $\bar\theta$, $\bar\Phi$ are the angles of the electron relative to the dipole axes. p is a variable parameter. The normalization was carried out in the usual manner requiring that $|C_0|^2 + |C_1|^2 = 1$.

The matrix element T_{fi} for the transition probability was calculated in the same manner as Turner. Simultaneous application of both corrections leads to the expression

$$T_{fi} = \frac{i\,D\,e\,m}{I K\sqrt{6\,p\,\pi}}\left\{(5\,\pi)^{1/2}\left[S_{fi}^{(1)} - \frac{2\,D\,e\,m}{3\,\hbar^2}\,\Delta S_{fi}^{(1)}\right] + \frac{(3\,\pi)^{1/2}}{2}\left[S_{fi}^{(3)} - \frac{4\,D\,e\,m}{3\,\hbar^2}\,\Delta S_{fi}^{(3)}\right]\right\}\left\{e^t E_i(-t) + e^{-t} E_i(t) + \frac{i\,\pi}{2}\,e^{-t}\right\}. \qquad (3)$$

Table 1.

Quantity	Turner's results	Values due to amplitude correction only	Values due to wave fn. correction only	Values due to simultaneous correction of both factors
Matrix element of the transition probability $\|T_{\mathrm{fi}}\|^2 \times 10^{-48}$	3.6	2.88	1.95	1.56
Life time of negative ion in sec $\times 10^{-13}$	1.3	1.72	3.024	3.78
Capture cross section in cm^2 $\times 10^{-14}$	2.4	1.92	1.299	1.0392

In expression (3) the corrections due to the variational approach to the scattering amplitude are

$$-\frac{2\,D\,e\,m}{3\,\hbar^2}\,\Delta S_{\mathrm{fi}}^{(1)} \quad \text{and} \quad -\frac{4\,D\,e\,m}{3\,\hbar^2}\,\Delta S_{\mathrm{fi}}^{(3)}$$

while the modification due to the use of Eq. (2) is

$$\left\{ e^{t}\,E_i(-t) + e^{-t}\,E_i(t) + \frac{i\,\pi}{2}\,e^{-t} \right\}$$

where t is equal to K/P. $S_{\mathrm{fi}}^{(1)}$; $S_{\mathrm{fi}}^{(3)}$; $\Delta S_{\mathrm{fi}}^{(1)}$; $\Delta S_{\mathrm{fi}}^{(3)}$ are defined in the appendix.

Considering an experiment at room temperature, with the help of Eq. (3) the calculations of the life time of a temporarily formed negative ion and the capture cross section are made exactly as Turner. The dipole moment D was taken to be 2×10^{-18} esu. cm. and I of the order of 10^{-40} gm. cm^2. In Table 1 results for the life time and capture cross section for the $L=2$ and $L=3$ states are exhibited.

It is observed that the correction term depends on the dipole moment and also on the velocity of the electron. The modification in the calculation is to increase the life time nearly three times and to decrease the capture cross section about 2.3 times.

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Appendix

The terms $S_{\mathrm{fi}}^{(1)}$; $S_{\mathrm{fi}}^{(3)}$; $\Delta S_{\mathrm{fi}}^{(1)}$; $\Delta S_{\mathrm{fi}}^{(3)}$ used in Eq. (3) are as follows.

$$S_{\mathrm{fi}}^{(1)} = L_f(L_f+1)\,[\alpha(L_i M_i)\,\delta_{L_f+1,\,L_i+1} + \beta(L_i M_i)\,\delta_{L_f,\,L_i-1}]\,\delta_{M_f M_i}$$

$$\Delta S_{\mathrm{fi}}^{(1)} = L_f(L_f+1)\,\delta_{L_f L_i}\,\delta_{M_f M_i}\,.$$

$$\begin{aligned} S_{\mathrm{fi}}^{(3)} = \{ & L_i(L_i-1)\,[\gamma(L_f M_f)\,\eta(L_i M_i) + \in(L_f M_f)\,\xi(L_i M_i)] \times \delta_{L_f+1,\,L_i-1} \\ & + (L_i+1)\,(L_i+2)\,[\gamma(L_i M_i)\,\eta(L_f M_f) + \in(L_i M_i)\,\xi(L_f M_f)]\,\delta_{L_f-1,\,L_i+1} \}\,\delta_{M_f M_i} \end{aligned}$$

$$\begin{aligned} \Delta S_{\mathrm{fi}}^{(3)} = {} & \tfrac{1}{3}\,[L_i(L_i+1) - 2]\,\delta_{L_f L_i}\,\delta_{M_f M_i} - \tfrac{1}{5}\,[L_i(L_i+1) - 4 + i] \\ & \{\alpha(L_i M_i)\,\delta_{L_f L_i+1} + \beta(L_i M_i)\,\delta_{L_f,\,L_i-1}\}\,\delta_{M_f M_i} + \tfrac{2}{5}\,\{L_i(L_i+1) \\ & + (M_i-2)\}\{\gamma(L_i M_i) + \eta(L_i M_i)\}[\in(L_f M_f)\,\sigma(L_i M_i)\,\delta_{L_f+1,\,L_i+2} \\ & - \in(L_f M_f)\,\varrho(L_i M_i)\,\delta_{L_f+1,\,L_i} + \xi(L_f M_f)\,\sigma(L_i M_i)\,\delta_{L_f-1,\,L_i+2} + \xi(L_f M_f)\,\varrho(L_i M_i)\,\delta_{L_f-1,\,L_i}]\,\delta_{M_f+1,\,M_i-1} \end{aligned}$$

were

$$\alpha(L,M) = \beta(L+1,M) = \left[\frac{(L+M+1)\,(L-M+1)}{(2\,L+1)\,(2\,L+3)}\right]^{1/2}$$

$$\gamma(L,M) = \eta(L+1,\,-M+1) = \left[\frac{(\mathrm{L}-M+1)\,(L-M+2)}{(2\,L+1)\,(2\,L+3)}\right]^{1/2}$$

$$\varrho(L,M) = \;= \sigma(L+1,M) = \left[\frac{(L+M)\,(L-M+2)}{(2\,L+1)\,(2\,L+3)}\right]^{1/2}$$

$$\in(L,M) = \xi(L+1,\,-M-1) = \left[\frac{(L+M+1)\,(L+M+2)}{(2\,L+1)\,(2\,L+3)}\right]^{1/2}.$$

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Scattering of Slow Electrons by Polar Molecules

H. S. Desai
Department of Physics, Faculty of Science
M S. University, Baroda
&
M. P. Maru
Department of Physics
H & H. B. Kotak Institute of Science, Rajkot

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The diffusion cross-section (Q_D) for electron scattering by a polar molecule is calculated by considering the molecule as a finite dipole. The assumption of a finite dipole instead of a point dipole in case of the H_2O molecule leads to a correction term to Q_D resulting in a value 0·3% less than that calculated using S. Altshuler's expression [*Phys. Rev.*, 107 (1957), 114].

THE calculation of diffusion cross-section or momentum transfer cross-section (MTCS) of electrons in polar molecules is very controversial. Several workers[1-3] have calculated MTCS for the low energy electrons of polar molecules, considering molecules as point dipoles. Recently Bordman and Sampnathe[4] have deduced a formula for the calculation of the cross-section by taking into account the screening effect due to the pressure of the gas. It seems that apart from the source of error due to the use of Born approximation, the concept of point dipole is also one of the sources of error. We have tried to estimate the error due to this approximation. The assumption of a finite dipole moment K instead of a point dipole (i.e. $K = 1$) leads to a correction term for the cross-section. This correction approximation, velocity-independent and the contribution given by this correction term is above 0·3%.

The expression for the potential $V(r)$ for the finite dipole in which two charges $+q$ and $-q$ are separated from each other by a distance $2a$ is

$$V(r) = -2eq \sum_{K=\text{odd}} \frac{r_{\min}^{K}}{r_{\max}^{K+1}} P_K(\cos\theta) \qquad \ldots(1)$$

where $r_{\min}$ and $r_{\max}$ are the minimum and the maximum values of r and $P_K(\cos\theta)$ is the Legendre polynomial. We shall consider the case $K = 1$; substituting this in an expression for Born approximation, we have for scattering amplitude:

$$f(\theta, \phi) = \frac{m}{2\pi\hbar^2}\left[\int_0^a\int_0^\pi\int_0^{2\pi} \frac{r}{a^2} e^{i\mathbf{K}\cdot r} P_1(\cos\theta)\, d^3r + \int_a^\infty\int_0^\pi\int_0^{2\pi} \frac{a}{r^2} e^{i\mathbf{K}\cdot r} P_1(\cos\theta)\, d^3r\right] \qquad \ldots(2)$$

where d^3r = volume element $= r^2 dr \sin\theta d\theta d\phi$.

On performing the elementary integration we get

$$f(\theta, \phi) = \frac{2iDem\gamma'}{\hbar^2 \mathbf{K}}\left[3\left(\frac{\sin \mathbf{K}a}{\mathbf{K}^3 a^3} - \frac{\cos \mathbf{K}a}{\mathbf{K}^2 a^2}\right)\right] \qquad \ldots(3)$$

where $D = 2aq$ and γ' is the direction cosine of the dipole axis with respect to the direction of $\boldsymbol{K}$; $\boldsymbol{K}$ is a wave vector, the magnitude of which is $K_0[2(1-\cos\theta)]^{\frac{1}{2}}$. It is observed that as $a \rightarrow 0$ the value of differential scattering cross-section coincides with the value calculated by Altshuler[1].

The diffusion or momentum transfer cross-section is given by

$$Q_D = \int (1-\cos\theta)\sigma_t d\Omega \qquad \ldots(4)$$

where σ_t = differential scattering cross-section.

Considering the target molecule as a rigid rotator, the calculation for Q_D is made in exactly the same way as Altshuler. The expression for Q_D is

$$Q_D = \frac{8\pi}{3}\left(\frac{Dem}{\hbar^2 K_0}\right)^2 [1 - 0{\cdot}4 K_0^2 a^2 + 0{\cdot}053 K_0^4 a^4] \qquad \ldots(5)$$

In Eq. (5) Q_D is given in cgs units which can be converted into πa_0^2 unit, where a_0 is the Bohr radius. The expression of Q_D in πa_0^2 unit is given by

$$Q'_D = \frac{Q_D}{\pi a_0^2} = \left[5{\cdot}6 \frac{(D')^2}{E'} - 0{\cdot}006579 (D')^4 + 0{\cdot}253 \times 10^{-5} (D')^6 E'\right] \qquad \ldots(6)$$

where

$$D' = \frac{D}{10^{-18}} \text{ units and } E' = \frac{E \times C}{10^8 e} \text{ in } \mathrm{V}^{1/2}$$

On comparing the result of Eq. (6) with that of Altshuler, it is seen that the correction due to finite dipole is

$$-0{\cdot}006579 (D')^4 + 0{\cdot}253 \times 10^{-5} (D')^6 E' \qquad \ldots(7)$$

For H_2O molecule this correction reduces the value of the cross-section as determined by Altshuler by 0·3%. Also, it can be seen that the correction depends more on the dipole moment than on the velocity of the electron.

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